DOE Workshop on Advanced Simulations:
A Critical Tool for Future Nuclear Fuel Cycles

LLNL, December 14-16, 2005

Session 2B

Neutronics Working Group

Chair: Forrest Brown

Abstract

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These slides provide introductory and background material for the working group session on "Neutronics". The session participants are expected to make short presentations on their own work, including possible impact on the design of future nuclear reactors. These will be followed by detailed discussion of how advanced simulation methods could contribute to the design of Generation-IV reactor systems. Based on the discussions, a technology roadmap for advanced reactor simulation will be proposed.

Advanced Simulations Workshop

- "… better understand the possible role of computer simulations within the nuclear energy program."

- "… want to understand what kinds of computational tools will need to be built … and the scale of resources that will be called for."

- **This working group: focus on NEUTRONICS**

Historical Perspective

- **TeraFlop computers are now common**
- **PetaFlop computers are coming, within 5 yr**
- **Parallel codes are routinely used at National Labs & some universities**

- **Commercial power reactor design & analysis is mainly performed on PCs, using "mature" codes**

- **What if parallel supercomputers were to be used?**
  - Benefits ?
  - Development needed ?
  - Technology Roadmap ?

Historical Perspective

- **Naval Reactors Program, 1980s**

  - New generation of 3D codes developed for supercomputers
  - Extensive historical database for verification & validation
  - Led directly to life-of-ship reactor designs in 1990s

- **DOE Advanced Simulation & Computing (ASCI)**

  - New generation of 3D parallel codes + TeraFlop computers
  - Integrated multi-physics codes, improved physics models
  - Stockpile stewardship, without nuclear testing

Historical Perspective - ASC

- **Software Development**
  - Large effort to develop new parallel algorithms & codes
  - Close interaction among code developers & users
  - Significant work on tools
    - Software development
    - Parallel debuggers
    - Visualization
    - Analysis tools
    - Batch queueing systems
    - Performance monitors
    - Equation solver packages
    - Grid generation
  - Software quality assurance
    - Extensive V&V effort
    - Adherence to SW standards
    - SW development methodology

- **Hardware Development**
  - Parallel TeraFlop systems
  - Data storage
    - High capacity
    - High bandwidth
  - High-speed networks

- **General**
  - Long-term plan, >10 year scope
  - Roadmap for technolgy, including milestones (deliverables)
  - Revise plans as needed, to match reality
  - $$$$$

Neutronics - Requirements

- **3-D whole-core calculation of current commercial PWR**

    50,000 fuel pins

    X 10 radial zones per pin

    X 100 axial zones

    X 300 isotopes per pin,

        plus fluxes & power

    ~ 120 GB per depletion point

    What new requirements are there for Gen-IV ?

- **Complete reactor analysis requires:**
    - 10,000s of steady-state 3-D core calculations
    - 100s of transient core calculations
    - 1000s of operational support calculations
    - Continuous real-time core monitoring calculations

- **Complications**
    - Economics
    - Fabrication tolerances
    - Uncertainties, unknowns, …

Neutronics - Methods

- **Current practice**
  - 2-D lattice physics codes
    - Multigroup transport
    - Largely a solved problem
    - 1000s of calculations per fuel bundle (depletion, Xe, B, temperature, …)
  - 3-D nodal codes
    - Parameterized few-group cross-sections from lattice codes
    - Need ~1% accuracy on pin powers
    - Pin power reconstruction
  - 3-D Monte Carlo
    - Primarily V&V at BOL

- **Current R&D**
  - 3-D transport, with explicit heterogeneous geometry
    - Must be parallel
    - Huge data storage reqmts
    - Need coupling to T/H codes
    - Currently too expensive for routine design work
  - Monte Carlo
    - Depletion (crude at present)
    - Temperature effects
    - Coupling to fluid codes
    - Parallel methods
    - Huge data storage reqmts
    - Currently too expensive for routine design work

Neutronics - Challenges

- **Neutronics codes must be fully coupled to thermal-hydraulics & other codes**
  - Must have consistent power, temperature, xenon, …
  - Also need to account for materials properties, fuel swelling, corrosion, …

- **Need to develop standard interface specifications**
  - May need to allow for "plug-in" of commercial proprietary code modules

- **Gen-IV reactor physics**
  - Different materials
  - Higher temperatures
  - Different (or no) moderator
  - Double heterogeneities
  - Different spectrum & burnup
  - V&V of new codes & methods

- **Developing new parallel codes for reactor analysis will take >5 yr**
  - Longer if new methods reqd
  - V&V will be huge effort

Neutronics - Roadmap

- **Requirements / Benefits**
  - What can't we do now ?
  - What can we do now that should be done better ?
  - What new requirements are there for Gen-IV ?

- **Timing**
  - How long will it take for new methods & parallel codes ?
  - How long will V&V take ?
  - How long to train users & overcome inertia ?
  - What impact will petaflop computers have ?

- **Roadmap**
  - Significant new capabilities vs time
  - Milestone calculations to demonstrate
  - Relation to other Gen-IV development

References

see website for PHYSOR-2004 plenary session:
www.physor2004.anl.gov/PlenarySessions.htm

(especially the talk by Kord Smith)

MCNP5 - Monte Carlo

- **30+ year history of continuous improvement by LANL X-Division**
- **The "gold standard" for neutronics calculations (shielding, criticality safety, reactors, …)**

- **Recent improvements**
  - Entropy of fission source distribution used to assess convergence in criticality calculations
  - Stochastic geometry for modeling VHTR fuel kernels
  - Automated method for temperature variations in cross-sections
  - Mesh tallies for editing power distribution & reaction rates
  - Linkage to T/H & depletion codes (U. Mich. & others)
  - ENDF/B-VII cross-section data

MCNP5 & Advanced Reactor Design

- **MCNP5 runs on nearly any parallel computer (using standard MPI & OpenMP)**

- **Depletion**
  - Possible now with MONTEBURNS linkage code, but many simplifications & limitations

- **Possible development for advanced reactors**
  - Improved, in-line depletion
  - Overcome storage limitations for very large reactor problems
  - Production features: equilibrium Xe, rod or B^{10} searches, …
  - Improved input & linkage to other reactor codes

MCNP5 & Advanced Reactor Design

- **Even with improvements & PetaFlop computers, MCNP may be too expensive to use for many 1000s of reactor design calculations**

- **Changes in design methodology may be needed**
  - Use MCNP for 3-D nominal depletion analysis
  - Calibrate 3-D deterministic transport code to MCNP
  - Use 3-D deterministic transport for off-nominal variations

  Use detailed 3-D Monte Carlo for "truth" calculation,

  Then use 3-D transport code for "delta" calculations